Investigation of conformational stability and vibrational spectra of halomethylsulfonyl isocyanates

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Abstract: The conformational behavior and structural stability of chloro- and fluoromethylsulfonyl isocyanates were investigated by quantum mechanical DFT and ab initio MP2 calculations. The 6-311++G(**) basis set was employed to include polarization and diffuse functions in the calculations. The molecules were found to exist in a mixture of two stable gauche conformations. The potential scans were calculated from which the rotational barriers could be estimated. The vibrational frequencies and spectra were computed at B3LYP/6-311++G(**) level. The potential energy distributions were then calculated to provide tentative vibrational assignment for the normal modes of the stable conformers of both molecules.